CHAPTER 1

Introduction

1-1. Opening Remarks.

a. The production of data of "known and acceptable quality" is a primary goal of every environmental restoration and compliance sampling effort. In general, some degree of data review should be performed for all data collection activities to help ensure that only scientifically defensible data are used to support project decisions. However, the extent of the review will be dependent upon the project's **data quality objectives (DQOs)** and will be limited by the physical contents of the data package.[1] For example, the reporting and evaluation requirements for **definitive data** and **screening data** will differ significantly.

b. This document provides guidance to the U.S. Army Corps of Engineers (USACE) and USACE contractors (e.g., to architect-engineering contractors and third-party data reviewers) for evaluating instrumental chemical data using a **performance-based approach**. A **performance-based method** is defined as an analytical procedure for which **data quality indicators** are documented and evaluated with respect to acceptance criteria that are established from project data quality objectives. In particular, the **PARCCS** parameters (i.e., **precision**, **accuracy**, **completeness**, **representativeness**, **comparability**, and **sensitivity**) are documented for the **target analytes** of concern at the levels of concern (i.e., at or below project action levels) in the environmental media of interest and are evaluated with respect to acceptance limits or **measurement quality objectives (MQOs)** that are designed to ensure that total measurement uncertainty is within the limits prescribed by project DQOs. This document assumes that DQOs and MQOs have been established and presents guidance for evaluating chemical data quality, as measured by PARCCS, as a *first step process* for data usability assessment. (Refer to Chapter 1.2.2 for additional discussion regarding data usability assessment.) [2] To more effectively assess data usability, it is recommended that existing data evaluation protocols and checklists be revised using at least some of the strategies presented in this document.

1-2. Scope and Limitations of Performance-Based Data Review.

a. In general, data packages must contain enough information to evaluate PARCCS.[3] Data packages must essentially contain summary results for instrument calibrations (initial and continuing), environmental samples, and associated **batch quality control (QC) samples** (e.g., **method blanks** and **laboratory control samples**), as well as select raw data. (Specific reporting requirements are addressed in Chapter 4 of this document.) Data packages that satisfy these reporting requirements will be referred to as **performance-based (PB) data packages** and the im-

[1]The definitions of a number of critical terms appear in bold print the first time they are used. These terms are defined in the body of the document or, more commonly, in the glossary at the end of the document. Italics are used to denote emphasis or special meaning.
[2]Since it is assumed that MQOs have been established and are consistent with DQOs, for simplicity, from hence forth, the distinction between the two terms will not be maintained; "DQOs" will also refer to the MQOs.
[3]Although this document constitutes guidance, terms such as "must," "shall," and "will" are used in the document when an item is viewed to be especially critical or when an activity is viewed to be typically appropriate.

plementation of the data evaluation activities described this document will be referred to as **performance-based (PB) data review.**

b. The data review protocols presented in this document should not be viewed as prescriptive algorithms but as strategies intended for the purposes of guidance. For example, quality control (QC) acceptance limits are specified in this document but these limits should be viewed as "baseline" limits that should be adjusted (i.e., increased or decreased) based upon the objectives of the project. Even if it were possible to specify a set of QC acceptance limits that would be applicable to all projects, the potential occurrence of multiple QC problems alone suggests that a prescriptive approach for data evaluation would be unfeasible (e.g., it would not be practical to propose an evaluation strategy for every combination of QC problems that could be encountered). Because of the complexities of environmental investigations and uniqueness of environmental samples, analytical data must ultimately be evaluated using **professional judgement** in the context of *project-specific data objectives*.

c. In order to successfully implement a PB review, the DQOs in project planning documents such as Work Plans, Sampling and Analysis (SAPs), and Quality Assurance Project Plans (QAPPs) must be well defined. The generation of DQOs is beyond the scope of this document. However, it should be noted that generic statements such as "definitive" or "Level IV data will be collected" will not suffice. A specific set of QC acceptance limits must be presented for the analytes of concern for the concentrations of interest for the environmental populations being sampled. In theory, project documents such as QAPPs contain comprehensive and appropriate QC specifications, but, in practice, this is not necessarily true (e.g., when the data reviewer is not adequately involved in the project planning process).

d. In order to perform a PB data review, project-specific data quality objectives must be scientifically defensible. The scientific defensibility of the data should take precedence over contract compliance issues or the QAPP when QAPP contains inappropriate specifications. For example, if the QAPP requires data to be evaluated solely upon the basis of method-specified QC criteria (e.g., such as those specified in SW-846 methods) or laboratory performance criteria, then the validity of assessing the data on this basis should be carefully evaluated before proceeding with the data review. In particular, sensitivity requirements should not be established solely on the basis of method-specified quantitation limits such as the Contract Laboratory Program (CLP) Contract Required Quantitation Limits (CRQLs). Method-specified quantitation limits may be inappropriately high for project-specific action levels (e.g., risk-based cleanup levels). Laboratory detection, quantitation, and reporting limits must be evaluated with respect to the project-specific action levels to demonstrate that the proposed analytical methods possess adequate sensitivity. Similarly, it would typically be inappropriate for the QAPP to establish method data quality objectives for precision and **bias** solely on the basis of a laboratory's statistical control limits (e.g., for **matrix spikes** and laboratory control samples). A laboratory's statistical limits may be indicative of the laboratory's routine performance but may be too wide to yield quantitatively reliable results.

e. Performance-based data review must not be performed as a "last-minute" activity that is initiated only after the completion of all sample collection and analysis. To the extent that is possible or practical, prior to performing a PB data review, the reviewer should possess a

complete understanding of the intended use of the data and the relationship of the QC results to the usability of the data. The reviewer must receive input from the end-data users regarding the objectives and expected results of the analyses (e.g., via the review of the Project Quality Assurance Plan and Sampling and Analysis Plan). For optimal results, the reviewer should be involved in the DQO process in the early planning stages of the project (e.g., should be involved in scoping meetings where project DQOs, scheduling, sampling techniques, analytical methodologies, and data evaluation criteria are established.) *When the data reviewer is not adequately involved in the DQO process, a PB data review may result in the rejection of a significant portion of the analytical data. Performance-based data evaluation strategies need to be specified during project planning*

1-2.1. Performance-Based Data Review Versus Data Validation.

a. This guidance is generally applicable to any instrumental performance-based method, regardless of the determinative or preparatory techniques used to process the environmental samples. The data review protocols will result in a relatively thorough evaluation of data quality and will be applicable to a variety of environmental projects. However, the data review strategies presented in this document may be insufficient for all data uses. Project-specific DQOs may require more comprehensive data evaluation activities than those performed during PB data review.

b. Performance-based data review does not constitute ***data validation****. Data validation* is a more in-depth evaluation of laboratory data quality and is beyond the scope of this document. As the term is used in this document, *data validation* refers to any independent systematic review of **comprehensive data packages** with respect to a predefined set of technical performance criteria for PARCCS. A *comprehensive data package* is defined as a data package that contains sufficient information to completely reconstruct the laboratory analyses that were performed and documents salient field sample collection and handling activities (e.g., contains the Chain-of-Custody and may contain field logs). Hence, comprehensive data packages contain summary data for environmental, **batch QC**, and **instrument QC sample** analyses as well as all the raw laboratory data (e.g., standard preparation logs and printouts of chromatograms). CLP data packages are examples of comprehensive data packages with distinct reporting requirements.

c. Data validation involves the evaluation of batch QC and calibration results, in addition to other instrument QC results using the raw data. Since all the raw laboratory data are not included in performance-based data packages (unlike for data validation), reported QC summary results (e.g., laboratory control sample and **surrogate** recoveries) are not verified to the level of the raw data (e.g., using chromatograms and other instrumental printouts). Furthermore, with the exception of calibration data, PB data packages do not contain instrument QC results (e.g., pesticide percent breakdown and tune checks). Hence, during PB data review, instrument performance (other than calibration) is assumed to be in control or out-of-control in a manner that is consistent with batch QC performance. This assumption is usually reasonable but is not always valid.

d. A more thorough data evaluation should be considered when significant QC problems are observed during PB data review or when data is being collected to support critical decisions. Since laboratories normally maintain files of all supporting data and documentation for the analyses performed (for the period of time that is normally specified in the contract for analytical services), the laboratory can be requested to provide copies of the raw data to perform a more comprehensive review when the need arises. However, it is recommended that requirements for archiving comprehensive data packages be explicitly addressed when contracting for analytical services.

e. During project planning, the objectives of the analyses, nature of the contamination, limitations of the analytical methodology, and historic information about the site should be evaluated to determine whether a more comprehensive review needs to be performed. In particular, if the analytical technique involves the use of a **2-D detector** rather than a **3-D detector**, then it is especially critical to take stability problems (e.g., photochemical and thermal degradation) and interferences into account when determining whether or not a more comprehensive evaluation is required. For example, a review of batch QC results alone would probably be inadequate to identify data quality problems when a high performance liquid chromatograph (HPLC) with a fluorescence detector is being used to measure low levels of polynuclear aromatic hydrocarbons (PAHs) such as benzo(a)pyrene at a site with high background fuel contamination. The evaluation of 4,4'-DDT and Endrin breakdown checks (e.g., as discussed in Method 8081A) may be required to determine whether or not **detections** of target analytes such as Endrin ketone and Endrin aldehyde are actually false positives arising from poor method implementation (e.g., the degradation of Endrin during instrumental analysis).

> Note: The evaluation strategies presented in this document may be less adequate for 2-D detector methods than 3-D detector methods. *However, this does not imply that the strategies are not appropriate or useful for 2-D detector methods.* The level of confidence for data will be a function of the nature of the analytical technique, regardless of the thoroughness of any data evaluation activity. It is merely being noted that, since 2-D methods inherently lack the specificity of 3-D methods, 2-D methods are more prone to data quality problems (e.g., false positives) that, under select circumstances, may only be identified via the evaluation of a full raw data package.

1-2.2. Performance-Based Data Review Versus Usability Assessment.

a. It is emphasized that the PB data review activities discussed in this document constitute only a first-step process for the assessment of data usability. A *full* assessment of data usability is a more complex and comprehensive activity than PB data review or validation; the former encompasses the latter and is potentially more subjective. The data user must ultimately assess the overall usability of data on the basis of *total measurement uncertainty* and the objectives of the investigation. .

b. Total measurement uncertainty consists of the sum of the *laboratory analytical uncertainty* and *field sampling uncertainty.* Unfortunately, *field sampling uncertainty* is often greater than *laboratory analytical uncertainty* and is not fully taken into account during data review or validation (i.e., data review and validation identify *laboratory analytical uncertainty* but do not

fully address *field sampling uncertainty)*. For example, data review and validation may identify incorrect preservation techniques but would not adequately characterize the representativeness of a sample collected from an environmental population with high spatial or temporal variability.

c. Little or no usability assessment is typically performed during data review or validation. Usability assessment is usually performed after data review or validation is completed. For example, when data validation is performed using the National Functional Guidelines, sensitivity is evaluated with respect to fixed CRQLs rather than project-specific action levels. However, meeting CRQLs does not ensure that the data will be usable (a problem which, unfortunately, many usability assessments also fail to identify). This document constitutes a more streamlined approach for data review. Data quality is evaluated during data review in the context of the end use of the data.

1-3. Overview of Performance-Based Data Review.

a. This section of the document presents a brief overview of the PB data review process. The reviewer initially receives input from the end-data users regarding the objectives and expected results of the analytical efforts (e.g., in the form of formal DQOs described in the Work Plan and QAPP). Prior to performing a PB data review, the reviewer performs a cursory evaluation of the data package to ensure that it contains all the required documentation. *This is critical since the evaluation of any data package will be limited by its physical content.* If the data package is essentially complete, the reviewer performs a more complete evaluation to determine if the data *potentially* meet the needs of the end user. The reviewer verifies that sample collection and handling activities were properly implemented in the field and subsequently evaluates the analytical quality of the laboratory data. A PB review includes the evaluation of the following QC elements:

(1) Completeness.

(2) Holding Time and Preservation.

(3) Initial Calibration.

(4) Initial Calibration Verification.

(5) Continuing Calibration Verification.

(6) Sensitivity (e.g., detection and quantitation limits).

(7) Blanks (e.g., field and method blanks).

(8) Laboratory Control Samples.

(9) Post-Digestion Spikes (for trace metal methods).

(10) Matrix Spikes.

(11) Matrix Spike Duplicates and Matrix Duplicates.

(12) Surrogates (for organic chromatographic methods).

b. Detailed definitions of these QC elements may be found in the USACE *Shell for Analytical Chemistry* and the glossary of this document.

c. Quality control samples are designed to evaluate the PARCCS parameters and identify quality problems in three specific areas: (i) Laboratory analytical performance, (ii) matrix effects, and (iii) field performance. For example, accuracy is assessed from calibration, laboratory control sample (LCS), matrix spike (MS), post-digestion spike (PDS), and surrogate data. Precision is evaluated from duplicate laboratory control and matrix spike samples. Sensitivity is evaluated using detection limits and quantitation limits. Representativeness is evaluated via the review of holding time and blank data. A laboratory's analytical performance is evaluated using calibration results (i.e., initial calibrations, initial calibration verifications, and continuing calibration verifications) and **batch QC samples** such as method blanks and laboratory control samples. Matrix effects are evaluated using matrix spike, surrogate spike, and post digestion spike recoveries**. Field duplicates**, **rinsate blanks**, and **trip blanks** are examples of QC samples that are used to assess QC problems associated with sample collection activities..

d. After (or during) the technical evaluation, the reviewer generates a **data review report** that summarizes the overall quality of the data and lists individual QC problems and any observations that may be relevant to the data's potential usability. Data review reports are discussed in Chapter 2.